Entanglement, combinatorics and finite-size effects in spin-chains

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We carry out a systematic study of the exact block entanglement in XXZ spin-chain at $\Delta = -1/2$. We present, the first *analytic* expressions for reduced density matrices of n spins in a chain of length L (for $n \leq 6$ and arbitrary but odd L) of a truly interacting model. The entanglement entropy, the moments of the reduced density matrix, and its spectrum are then easily derived. We explicitely construct the "entanglement Hamiltonian" as the logarithm of this matrix. Exploiting the degeneracy of the ground-state, we find the scaling behavior of entanglement of the zero-temperature mixed state.

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Introduction. Entanglement is a central concept in quantum information science and it is becoming a common tool to study and analyze extended quantum systems because of its use in detecting the scaling behavior close to a quantum critical point [1]. It is has been pointed out that this scaling behavior is connected with the efficiency of numerical methods as quantum and density matrix renormalization group (DMRG) [1].

Let ρ be the density matrix of a system and let the Hilbert space be written as a direct product $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$. A's reduced density matrix is $\rho_A = \mathrm{Tr}_B \rho$ and the entanglement entropy is the corresponding Von Neumann entropy

$$S_A = -\mathrm{Tr}_A \rho_A \log \rho_A \,, \tag{1}$$

and analogously for S_B. When ρ corresponds to a pure quantum state $S_A = S_B$.

When A is a segment of length n of an infinite one-dimensional system in a critical ground state, the corresponding entanglement entropy S_n diverges as the logarithm of the sub-system size [2, 3, 4]

$$S_n = \frac{c}{3} \log n + c'_1 \,, \tag{2}$$

where c is the central charge of the associated conformal field theory (CFT) and c'_1 a non-universal constant. Away from the critical point, S_n saturates to a constant [3] proportional to the logarithm of the correlation length [4]. These properties made the entanglement entropy a basic tool to analyze 1D models. While it is impossible to mention here all the important contributions in the field, we refer the interested reader to the reviews [1].

In recent times, it has been remarked by few authors [5, 6] that the reduced density matrix ρ_n contains much more information than S_n. To the best of our knowledge the full reduced density matrix is known only for free systems [7] and is difficult to be obtained by numerical methods because these tend to focus on its eigenvalues. In order to go beyond free systems and to study the effect of strong interactions, in this letter we report a first systematic study of the reduced density matrix of the antiferromagnetic XXZ chain at $\Delta = -1/2$ defined by the Hamiltonian

$$H = -\sum_{j=1}^{L} [\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + \Delta \sigma_j^z \sigma_{j+1}^z] \,, \tag{3}$$

with periodic boundary conditions ($\sigma_{L+1} = \sigma_1$) and an odd number of sites. Here $\sigma_i^{x,y,z}$ stand for the Pauli matrices at the site i. This critical model has the unique property that all the components of the ground-state wavefunction are integer multiples of the smallest one [8]. We will argue in the following that this property suffices to get $\rho_n(L)$ for $n \leq 6$ and arbitrary L: an exceptional result for a truly interacting system. Another unique feature of this spin-chain is that the ground-state energy, which is doubly degenerate for any finite L has no corrections to scaling: $E_0 = -(3/2)L$ exactly. We refer to the two ground states as $|\Psi_\pm\rangle$ with the upper index being the sign of the total spin in the z-direction.

This work is complementary to two recent papers. In Ref. [9] ρ_n has been calculated in the thermodynamic (TD) limit (also for n up to 6). In Ref. [10] the connection with loop-models has been explored, for a different measure of entanglement. In contrast, here the emphasis is on combinatorial and finite-size scaling aspects. The exact value of some elements of the reduced density matrix for smaller values of n is also known for general Δ [11] and all of them up to $n = 6$ for $\Delta = -1$ [12].

Analytic results for ρ_n. Since the ground-state energy is exactly proportional to the system size, and the Hamiltonian is represented by a matrix with rational elements, also the ground-state vector has only rational components. Suitably normalized, all ground-state components are integer multiples of the smallest one. The ground-state for system sizes up to $L = 25$ can be then obtained with absolute precision in very modest computer time. With these ground-states we can construct the corresponding density matrices $\rho_n(L)$ with $n \leq L$. Any element of $\rho_n(L)$ is necessarily a rational number and in fact a rational function of L, with numerator and denominator of degree $\lceil n^2/2 \rceil$. The data suffice to guess the denominator to be $2^{n^2} L^n \prod_{k=1}^{\lfloor n/2 \rfloor} (L^2 - 4k^2)^{n-2k}$. (Anti)symmetrized with respect to the two ground states

$\rho_n(L)$ turns out to be an even (odd) function of L. As a result it can be determined completely for general L and for $n \leq 6$. For example, for $n=1$ and $n=2$ we obtained

$$\rho_1(L) = \frac{1}{2L}\begin{pmatrix} L+1 & 0 \\ 0 & L-1 \end{pmatrix}, \tag{4}$$

$$\rho_2(L) = \frac{1}{2^4 L^2} \times \tag{5}$$
$$\begin{pmatrix} 2(L+2)^2-2 & 0 & 0 & 0 \\ 0 & 6L^2-6 & 5L^2+3 & 0 \\ 0 & 5L^2+3 & 6L^2-6 & 0 \\ 0 & 0 & 0 & 2(L-2)^2-2 \end{pmatrix}.$$

The other reduced density matrices are too large to display. We enclose an electronic Mathematica file (the density matrix is `rho[L,n]` with L odd and $n=1,\cdots,6$). In the mathematica file and in the following, the indeces of the matrix are the decimal form of the binary number representing the site product state (1 for + and 0 for −).

We observed the following properties of ρ_n:
(i) The first and the last elements correspond to the probability of a string of equal spins, i.e. the emptiness formation probabilities (EFP), $E_\pm(L,n)$, which is

$$\prod_{k=0}^{n-1} \frac{k!\,(3k+1)!\,(L-k-1)!\,(\frac{L\pm1}{2}+k)!}{(2k)!\,(2k+1)!\,(L+k)!\,(\frac{L\pm1}{2}-k-1)!} \tag{6}$$

for minority (see [8]) and majority spins respectively. These two elements approach the same limit as $L\to\infty$, and are equal to $\rho[1,1] = A_n/2^{n^2}$, where A_n is the number of $n \times n$ alternating sign matrices (ASM).
(ii) Some elements satisfy relations that connect ρ_n to ρ_{n-1} when summing over one spin (see the appendix A of Ref. [9]). These equations can be used to derive expressions for some more elements. For example, we have $\rho_{n+1}[1,1] + \rho_{n+1}[2,2] = \rho_n[1,1]$, that combined with the ASM sequence for $\rho_n[1,1]$, gives $\rho_n[2,2] = (2^n A_{n-1} - A_n)/2^{n^2}$. Similar relations can be derived for a few other elements.
(iii) For $L\to\infty$ all non-zero elements remain non-zero and reproduce the results of Ref. [9].
(iv) The analytic continuation to general L satisfies $\rho_n(L)[i,j] = \rho_n(-L)[2^n+1-i, 2^n+1-j]$.

The entanglement entropy in the TD limit is

$$\begin{aligned} S_1 &= \log 2, \quad S_2 = 0.950749, \quad S_3 = 1.09287, \\ S_4 &= 1.19076, \quad S_5 = 1.26588, \quad S_6 = 1.32701 \end{aligned} \tag{7}$$

the same as in Ref. [9]. We are in position to study the finite-size effects. In Fig. 1 we plot $S_n(L) - 1/3\log L/\pi$, and we compare it with the CFT prediction [4] $1/3 \log\sin(\pi n/L) + c'_1$ valid for large enough n. We notice that all the results fall on the same curve, except for small deviations at $n=1$. It is impressive and maybe unexpected that the asympotic scaling sets in for such small value of n.

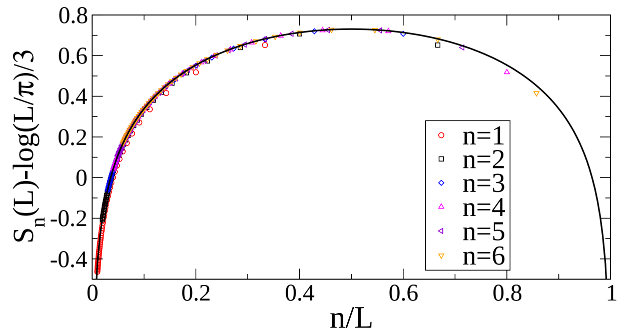

FIG. 1: Finite size scaling of the entanglement entropy $S_n(L)$ against the CFT prediction $1/3 \log\sin(\pi n/L) + c'_1$ (full line). We fixed $c'_1 = 0.7305$ [13].

Combinatorics. It has been noted in the study of Hamiltonian (3) that many physical quantities are sequences of integers or rationals that can be recognized in terms of known ones, with the ASM sequence for the ground-state components that is the best known [8], but not the only one [8, 15, 16].

Once a sequence has been recognized, the critical exponents can be derived exactly from its asymptotic behavior, which in part motivates the great interest in this kind of studies. One could have hoped that the eigenvalues of the reduced density matrices are rational or at least simple functions of L, but this is not the case. It is then natural to move our attention to the elements of the density matrix itself. Because of the conservation of the spin in the z direction, the density matrix has non zero entries only between states with the same magnetization ($= -n/2, -n/2+1, \ldots n/2-1, n/2$) and organizes into sectors, as evident from the block structure above. We already reported the formula for the first and last element of $\rho_n(L)$, that are the only elements in the sectors with spin $\pm n/2$. For the other sectors, the elements grow too quickly with n to recognize any simple behavior. For this reason we explored the possibility that some non-trivial combinations of them could have a simpler structure. Let us start by considering the sectors with total spin $\pm(n/2-1)$. After some tries, we found that reasonable growing sequences are given by the trace of the matrix multiplied with the matrix $(-1)^{i+j}$. In the TD limit, this results in the following sequence:

$$1,\ 2,\ 11,\ 72,\ 806,\ 14352, \tag{8}$$

for both sectors, up to an overall factor 2^{-n^2}. This sequence grows with n mildly, but we have been unable to recognize it. At finite L, the same trace for $\rho_n(2n+1)$ gives

$$\begin{aligned} &1,\ 2,\ 31,\ 124,\ 489,\ 1826,\ 6843,\ 25712,\ 97213, \\ &\quad 369478,\ 1410831,\ 5408272, \end{aligned} \tag{9}$$

$$\text{and}\ \ 2,\ 2,\ 2,\ 2,\ 2,\ 2,\ 2,\ 2,\cdots \tag{10}$$

for the two sectors with $S_z = \pm(n/2-1)$ of $\rho_n(2n+1)$ respectively, up to the overall factor $E_-(2n+1,n)$ from Eq. (6). The first sequence also grows in a reasonable way, but still we have not been able to guess it. For second one, the recognition is instead obvious and provide a non-trivial relation whose physical origin is still unknown. Similar sequences are easily derived for the other sectors. We want to stress here that this generation of sequences is not only an academic game. If we would have been able to find a sufficient number combinations of elements of the reduced density matrix that can be recognized, we would have been access to analytic forms of the reduced density matrix for any n and L. By simply looking at the elements of the density matrix this could seem an impossible task, but we explicitly showed that at least one combination of them is very easy and that there are other sequences that do not look prohibitive. The main reason why we reported these series here is to stimulate further studies in this direction in order to eventually achieve the knowledge of the full density matrix.

The moments of $\rho_n(L)$

$$R_n^{(\alpha)}(L) = \mathrm{Tr}\,\rho_n^\alpha(L)\,, \tag{11}$$

for α integer are sequences of rationals. For critical systems they display the universal asymptotic behavior [2, 4]

$$R_n^{(\alpha)}(L) = c_\alpha \left[\frac{L}{\pi}\sin\frac{\pi n}{L}\right]^{-c(\alpha-1/\alpha)/6}, \tag{12}$$

from which one can reconstruct the full spectrum of $\rho_n(L)$ [6] and its behavior is connected with the accuracy of some numerical algorithms based on matrix product states [17]. Despite this universal behavior $R_n^{(\alpha)}$ has been only marginally considered in the literature [4, 18]. In the TD limit, since all elements of $\rho_n(\infty)$ have a common denominator 2^{n^2}, all moments can be written as

$$R_n^{(\alpha)} = r_n^{(\alpha)}\, 2^{-\alpha n^2}, \quad \text{with } r_n^{(\alpha)} \text{ integers.} \tag{13}$$

For example, the values of $r_n^{(2)}$ up to $n=6$ are

$$\begin{aligned} &r_1^{(2)} = 2, \quad r_2^{(2)} = 130, \quad r_3^{(2)} = 107468, \\ &r_4^{(2)} = 1796678230, \quad r_5^{(2)} = 413605561988912, \\ &r_6^{(2)} = 1768256505302499935380\,. \end{aligned} \tag{14}$$

We are not able to recognize this fast growing sequence. Increasing α, the growth is even faster.

The numerical values of $R_n^{(2)}$:

$$\begin{aligned} &R_1 = 0.5, \quad R_2 = 0.507813, \quad R_3 = 0.409958, \\ &R_4 = 0.418322, \quad R_5 = 0.367356, \quad R_6 = 0.374443. \end{aligned} \tag{15}$$

clearly display even-odd oscillations that prevent us from any precise scaling analysis as the previous one for the entropy. Multiplying this by $n^{1/4}$ (see Eq. (12)) we get

$$0.5, \quad 0.604, \quad 0.540, \quad 0.592, \quad 0.549, \quad 0.586, \tag{16}$$

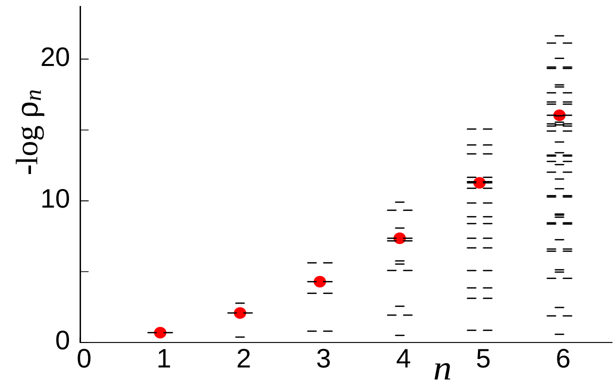

FIG. 2: Spectrum of ρ_n in the TD limit, the dots represent the first and last element Eq. (6). Note that these dots sit at 3/4 (2/3) of the spectrum for odd (even) n.

that tend to approach a constant value confirming the CFT scaling. A systematic study of these oscillations requires the analysis of larger values of n, that are not accessible to the present method and for which we performed DMRG calculations that appear elsewhere [14]. For periodic boundary conditions, these oscillations are only present for $\alpha \neq 1$, and not for the entanglement entropy. Thus they have a different origin than those found elsewhere for S_n that are due to boundary effects [19, 20]. The same kind of oscillations have been found numerically for the multi-interval entanglement [21]. It is rather natural that all the elements of $\rho_n(L)$ oscillate as a consequence of the tendency to antiferromagnetic order of the XXZ chain at $\Delta = -1/2$, and consequently most of the averages that are calculated from them are expected to oscillate as the moments do. Why and how these oscillations cancel between each other only for the von Neumann entropy is still mysterious.

$R_n^{(\alpha)}$ is not the only scaling quantity that can be represented as sequence of rationals. A good alternative is given by the central values $Q_n^{(\alpha)} \equiv R_n^{(\alpha)}(2n+1)$, which grows more slowly. In fact, in the matrix $\rho_n(2n+1)$ the common denominator is the inverse of $E_-(2n+1,n)$ in Eq. (6). As a typical example we report $Q_n^{(2)} = q_n E_-^2(2n+1,n)$:

$$\begin{aligned} &q_1 = 5, \ \ q_2 = 327, \ \ q_3 = 159502, \ \ q_4 = 680263760, \\ &q_5 = 22821555833635, \ \ q_6 = 6408136183930928388\,. \end{aligned} \tag{17}$$

Unfortunately, although it grows slower than $r_n^{(2)}$, we are also unable to recognize the sequence, but the guessing seems less prohibitive.

The spectrum of ρ_n in the TD limit is shown in Fig. 2. Several interesting features are evident in the plot. For odd n all the eigenvalues are doubly degenerate, while for even n only some. The spectrum at n is roughly repeated at the bottom and at the top of the spectrum at $n+2$ with some new structure in between. This is also

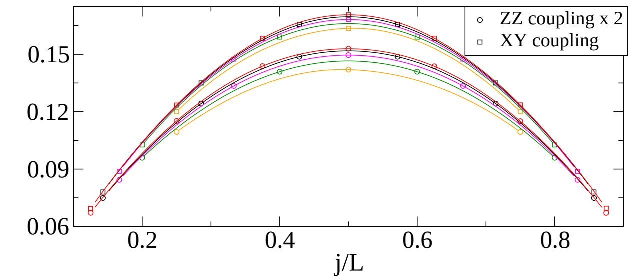

FIG. 3: Dependence of the coupling constants of the entanglement Hamiltonian on the position in the block. Squares (circles) refer to the XY (2 times ZZ) couplings, while the full lines are only guides for the eyes to connect points at the same n.

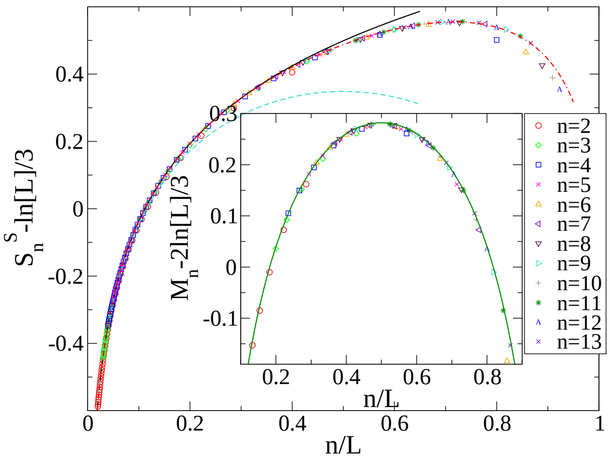

FIG. 4: Entanglement entropy of the symmetrized density matrix $S^s_n(L)$ versus n/L and its asymptotic behavior. The full line is $(\log n)/3 + c'_1$ that is an effective description up to $n/L \sim 0.5$. The dashed line is the finite-size CFT prediction for pure state $(\log L/\pi \sin \pi n/L)/3 + c'_1$ that clearly does not work for $x \geq 0.2$. The dashed-dotted curve is the heuristic formula $S^{(s)}_n(L = n/x) \simeq 1/3 \log\left[n(1 - A\sinh^4 x)\right]$ with $A \simeq 0.48$ that works well for all values of n (except very small n and $L - n$). Inset: Scaling of the mutual information M_n as function of n/L compared with the symmetrized heuristic guess.

what happens for free fermions [7] ($\Delta = 0$ in Eq. (3)). Thus the interaction appears to change only quantitative features of the spectrum and not the qualitative ones. This is highly non-trivial because non-zero Δ introduces well-known strong non-perturbative effects. The smallest eigenvalue scales like const$^{n^2}$ (i.e. the top of Fig. 2 is almost a parabola). Such scaling is known to be true for the "all up" eigenvalue $\rho[1, 1]$, i.e. to the EFP [16], that is marked as a dot in the figure.

The logarithm of the density matrix can be interpreted as an effective Hamiltonian for the subsystem through the natural definition $\rho_n(L) = e^{-\hat{H}_n(L)}$ at a fictitious temperature $T = 1$ (as observed independently [5]). This effective Hamiltonian can be written down exactly only for free fermions [7], but it is extremely difficult to obtain even part of it for interacting systems, because it requires the knowledge of the full density matrix. The present study gives this unique opportunity (it is enough to diagonalize the density matrix, taking the logarithm of the eigenvalues and then use the diagonalizing transformation to go back to the original spin basis). In the TD limit we find that the largest terms are a diagonal interaction, $J^z_j S^z_j S^z_{j+1}$, and a nearest neighbor exchange $J_j S^+_j S^-_{j+1}$+hc with a ratio ~ -0.55 that is almost the same as in the original model -0.5. All other terms (exchanges over larger distance, exchange of more than one pair of spins, multispin interaction) are more than one order of magnitude smaller. The couplings depend on the position roughly quadratically

$$J^z_j(n) \simeq A\frac{j(n-j)}{n}\,, \tag{18}$$

with $A \sim 0.6$. The parabolic dependence of the coupling constants is shown in Fig. 3.

The symmetrized density matrix. The degeneracy of the ground-state at finite L gives another unique opportunity: the symmetrized density matrix

$$\rho^s = \frac{1}{2}(|\Psi_+\rangle\langle\Psi_+| + |\Psi_-\rangle\langle\Psi_-|)\,, \tag{19}$$

corresponds to minimum energy and it is a zero temperature mixed state. ρ^s has no interpretation in CFT, and so it is a new quantity. In the TD limit $S(\rho^s_n) = S(\rho_n)$. In Fig. 4 we report the exact results for the entanglement entropy $S^s_n(L)$ of this mixed state. Up to $n/L \sim 0.5$ they are well described by $S^s_n(L) = (\log n)/3 + c'_1$, (*independent* of L and with the same c'_1 as before) as shown by the full line in the plot. Note that a finite size correction in the form of a sine (dashed-line) does not work for $x > 0.2$. However, a good collapse is observed for all x. (the last points that do not fall on the master curve correspond to $n = L - 1$ and are not expected to scale). We find that the corrections to the $\log n$ behavior are of the order of $(n/L)^4$. The collapsed data are fit remarkably well by $S^{(s)}_n(L = n/x) \simeq 1/3 \log\left[n(1 - A\sinh^4 x)\right]$ with $A \simeq 0.48$. We do not claim that this form has any justification.

In a mixed state the entropy (1) is not a good measure of entanglement because it mixes classical and quantum correlations. From quantum information we know that an appropriate measure is the mutual information

$$M_n = S_n + S_{L-n} - S_L\,. \tag{20}$$

The calculation of M_n is more difficult because even for small n we need S_{L-n} that can correspond to a large block. The data available from the exact ground state (up to $n = 13$, $L = 21$ plotted in the inset of Fig. 4) collapse and define a universal function that is described by the symmetrized version of the heuristic $S^{(s)}_n(L)$ in-

troduced before, plotted as a full line in Fig. 4.

Such mixed zero-temperature states are present every time that the ground-state is degenerate at finite L. Among these, supersymmetric lattice models [22] are very interesting and they could be understood more deeply in this framework.

Conclusions and perspective. We presented explicit analytic expressions for the reduced density matrix of the XXZ spin-chain at $\Delta = -1/2$. From these matrices we built several sequences of integers that encode the scaling behavior. From the exact density matrix, we constructed the entanglement Hamiltonian, a result that is not easily accessible to other approaches. We found the remarkable property that this Hamiltonian is dominated by nearest-neighbor terms of the same form as the original Hamiltonian. Finally, because the ground-state is doubly degenerate, we could study the entanglement of a zero-temperature mixed state, showing a very different behavior from a pure one.

These results are unique in two ways: they concern the full density matrix rather than only its entropy, and they are completely exact rather than asymptotic. They suggest many questions that can be posed also numerically for more general systems. They show explicitly that even for modest block size, asymptotic behavior is evident, eventually allowing for the study of further finite size corrections. Finally, since the ground state is known to have strong connections with combinatorial problems of current interest [8, 10, 15, 16], it is expected that further properties of the density matrix for arbitrarily large blocks can be found by combinatorial methods.

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